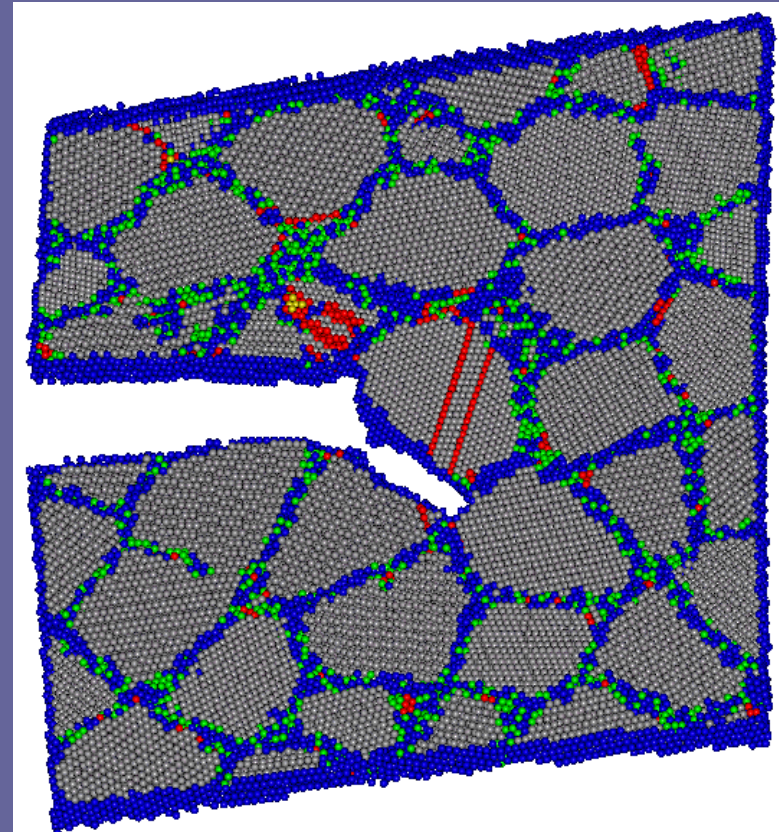


Computer Simulation of Fracture and Deformation Behavior of Nanocrystalline
Metallic Materials, DMR award number # DMR 9753243,
Diana Farkas, Department of Materials Science and Engineering,
Virginia Tech, Blacksburg, VA

The research is a fundamental investigation of the mechanisms of fracture and deformation in nanocrystalline materials. We have simulated intergranular fracture in nanocrystalline Ni modeled using fully 3D atomistic techniques. The crack advances by the formation of micro-voids ahead of the main crack. This year we have performed (1) a detailed analysis of the morphology of the propagating crack and the spatial distribution of the intergranular nano-voids formed ahead of the crack and its correlation with the local hydrostatic pressure distribution at the crack tip, and (2) a detailed analysis of the dislocation activity, demonstrating that full dislocations and twinning are observed around the crack tip in agreement with the experimental in-situ experiments.



Crack advancing in a 3D sample of nanocrystalline Ni, showing dislocation activity and twinning

Educational:

The research results are incorporated into our curriculum in the teaching of basic computer simulation techniques and mechanical behavior of materials. During this past year lectures series were given in two graduate classes at MIT and one at Brown University, during a sabbatical stay by the PI at those institutions.

Collaborators:

H. van Swygenhoven (PSI,
Switzerland)

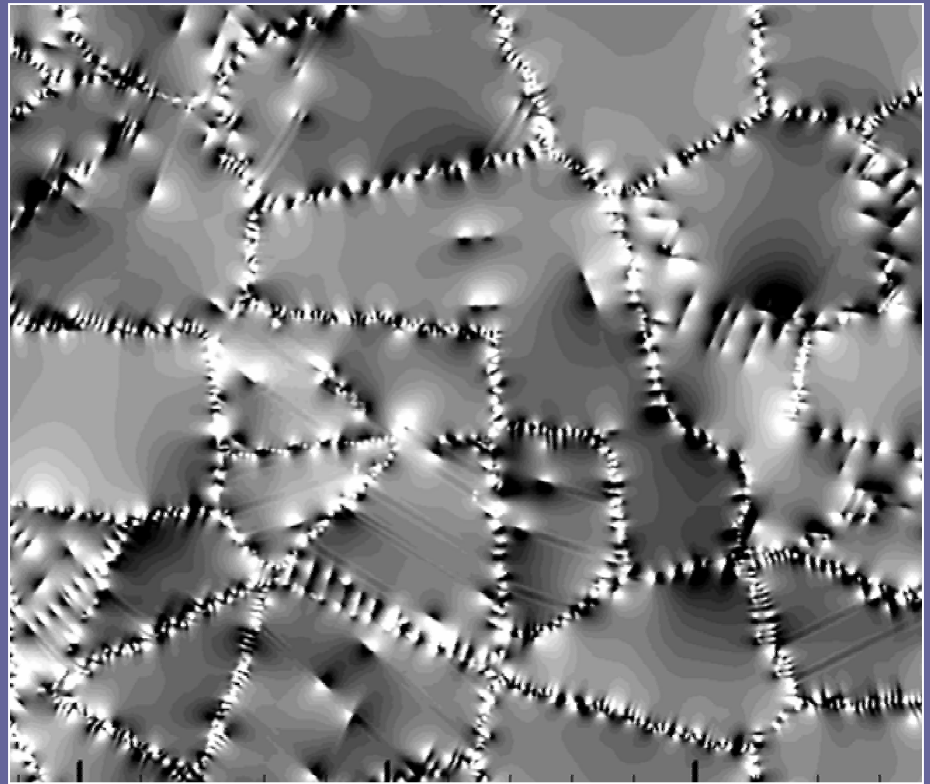


Illustration of dislocation activity in nanocrystalline Ni under tensile deformation used in teaching graduate classes in defect structure and mechanical behavior